Formic acid, (3-phenoxyphenyl)methyl ester

Inchi: InChI=1S/C14H12O3/c15-11-16-10-12-5-4-8-14(9-12)17-13-6-2-1-3-7-13/h1-9,11H,10H2
InchiKey: MJRCKLQMGSPMPF-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: O=COCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-27.33	kJ/mol	Joback Method
hf	-220.72	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.152		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1842.00		NIST Webbook
tb	671.56	K	Joback Method
tc	906.34	K	Joback Method
tf	399.36	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.61	J/mol×K	671.56	Joback Method
cpg	455.00	J/mol×K	710.69	Joback Method
cpg	468.30	J/mol×K	749.82	Joback Method
cpg	480.54	J/mol×K	788.95	Joback Method
cpg	491.74	J/mol×K	828.08	Joback Method
cpg	501.93	J/mol×K	867.21	Joback Method
cpg	511.13	J/mol×K	906.34	Joback Method
dvisc	0.0010846	Pa×s	399.36	Joback Method
dvisc	0.0006374	Pa×s	444.73	Joback Method

dvisc	0.0004133	Pa×s	490.09	Joback Method
dvisc	0.0002884	Pa×s	535.46	Joback Method
dvisc	0.0002129	Pa×s	580.83	Joback Method
dvisc	0.0001642	Pa×s	626.19	Joback Method
dvisc	0.0001312	Pa×s	671.56	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume